

Nonequilibrium current driven by a step voltage pulse: an exact solution

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One of the most important problems in nanoelectronic device theory is to estimate how fast or how slow a quantum device can turn on/off a current. For an arbitrary noninteracting phase-coherent device scattering region connected to the outside world by leads, we have derived an exact solution for the nonequilibrium, nonlinear, and time-dependent current driven by both up- and down-step pulsed voltages. Our analysis is based on the Keldysh nonequilibrium Green's functions formalism where the electronic structure of the leads as well as the scattering region are treated on an equal footing. A model calculation for a quantum dot with a Lorentzian linewidth function shows that the time-dependent current dynamics display interesting finite-bandwidth effects not captured by the commonly used wideband approximation.

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Understanding coherent transport of charge and spin through the scattering region of a nanoscale device is the central problem of nanoelectronics theory which has tremendous scientific and technological importance [1]. From both theory and application points of view, an important issue which has yet to be resolved is to predict how fast or how slow a nanoelectronic device can turn on/off a current from quantum mechanical first principles. Indeed, one cannot develop an electronic technology unless the operational speed of the device can be designed and controlled. This issue is closely related to the transient transport phenomenon, which is becoming an extremely important problem of nanoelectronic device physics, as can be observed in such effects as photon-assisted tunneling [2], electron turnstiles [3] and ringing behavior in the time-dependent current [4, 5]. Recent real-time measurements of electron dynamics [6] have further raised interest for the study of transient quantum transport.

The purpose of this work is to investigate transient quantum transport far from equilibrium, for nanoelectronic systems in the Lead-Device-Lead (LDL) configuration where “Device” indicates the scattering region which is connected to the outside world by the leads. When the LDL system is driven far from equilibrium by a step-shaped voltage pulse, we discovered an *exact* solution to the time-dependent current $J(t)$, thereby an *exact* transient quantum transport picture is obtained. To the best of our knowledge, this is the first time an exact solution is found for far-from-equilibrium transient transport dynamics in the quantum regime, and it provides a valuable and unambiguous physical picture of how charge current is turned on and off by a bias voltage pulse through devices of the LDL form. Importantly, the exact solution provides, for example, the correct current decay time scale after the bias voltage is turned off, and the transient current that follows the turning-on of a constant voltage.

For quantum devices in the form of LDL, the theoretical formalism best suited to the study of time-dependent transport is, perhaps, the Keldysh nonequilibrium Green's functions [4, 5]. In the NEGF formalism, the time-dependent current through the phase-coherent scattering region of the device is given in terms of local Green's functions. However, these Green's functions cannot, in general, be solved analytically. Previous studies of time-dependent transport have thus so far relied on the so-called wideband limit (WBL) [7], which is a simplifying assumption where the coupling between the scattering region and the external leads is taken to be independent of energy. In other words, the WBL neglects any electronic structure of the device leads. Therefore, when the electronic structure of the leads is important, *i.e.* for leads with finite bandwidth such as those made of semiconductors, nanotubes, nanowires, etc., a theory beyond the WBL is necessary. In this regard, *numerical* approaches have been put forward in Refs. 8, 9.

Our starting point is the formalism described in Refs. 4, 5, 10. The Hamiltonian of the LDL device is

$$H = \sum_{\mathbf{k}\alpha} \epsilon_{\mathbf{k}\alpha}(t) c_{\mathbf{k}\alpha}^\dagger c_{\mathbf{k}\alpha} + \sum_{mn} \epsilon_{mn}(t) d_m^\dagger d_n + \sum_{\mathbf{k}\alpha,n} \left(t_{\mathbf{k}\alpha,n} c_{\mathbf{k}\alpha}^\dagger d_n + t_{\mathbf{k}\alpha,n}^* d_n^\dagger c_{\mathbf{k}\alpha} \right), \quad (1)$$

where $c_{\mathbf{k}\alpha}^\dagger$ ($c_{\mathbf{k}\alpha}$) with $\alpha = L, R$ creates (destroys) an electron with momentum \mathbf{k} in the left (L) or right (R) lead, and d_n^\dagger (d_n) creates (destroys) an electron in a single-particle state labeled by n in the scattering region. Quantities $t_{\mathbf{k}\alpha,n}$ describe coupling of the leads to the scattering region of the device. Chemical potentials in both leads are set to zero. As in Refs. 4, 5, 10, when an external time-dependent voltage is applied to drive a current through the device, we assume that the single-particle energies acquire a time-dependent shift: $\epsilon_{\mathbf{k}\alpha}(t) = \epsilon_{\mathbf{k}\alpha}^0 + \Delta_\alpha(t)$ and $\epsilon_{mn}(t) = \epsilon_{mn}^0 + \Delta_{mn}(t)$. It has

been shown [5] that the charge current through lead α is given by

$$J_\alpha(t) = -2e \int_{-\infty}^t dt' \int \frac{d\epsilon}{2\pi} \text{Im Tr} \{ e^{i\epsilon(t-t')} e^{i \int_{t'}^t dt_1 \Delta_\alpha(t_1)} \times \Gamma_\alpha(\epsilon) [G^<(t, t') + f(\epsilon) G^R(t, t')] \}, \quad (2)$$

where $f(\epsilon) \equiv (e^{\beta\epsilon} + 1)^{-1}$ is the Fermi function, the linewidth function $\Gamma_\alpha(\epsilon)$ has matrix elements $\Gamma_{\alpha,mn}(\epsilon) \equiv 2\pi\rho_\alpha(\epsilon)t_{\alpha,m}^*(\epsilon)t_{\alpha,n}(\epsilon)$ where $\rho_\alpha(\epsilon)$ is the density of states in lead α , the lesser Green's function $G^<(t, t')$ has matrix elements $G_{nm}^<(t, t') \equiv i\langle d_m^\dagger(t')d_n(t) \rangle$ and the retarded Green's function $G^R(t, t')$ has matrix elements $G_{nm}^R(t, t') \equiv -i\theta(t-t')\langle \{d_n(t), d_m^\dagger(t')\} \rangle$. The retarded Green's function is given by the solution of the Dyson equation [10, 11] $G^R(t, t') = G_0^R(t, t') + \int dt_1 \int dt_2 G_0^R(t, t_1) \Sigma^R(t_1, t_2) G^R(t_2, t')$, where $G_0^R(t, t')$ is the Green's function of the scattering region without any leads, while the Keldysh equation yields the lesser Green's function $G^<(t, t') = \int dt_1 \int dt_2 G^R(t, t_1) \Sigma^<(t_1, t_2) G^A(t_2, t')$, where $G^A(t, t')$ is the advanced Green's function and $\Sigma^{R,<}(t_1, t_2)$ are the retarded and lesser self-energies, respectively. From a mathematical point of view, the main effect of broken time-translational invariance due to the presence of time-dependent external fields is that the double integral Dyson equation is not a simple Fourier convolution product as is the case in equilibrium or for steady-state transport, and therefore cannot be reduced by a Fourier transformation to a simple algebraic matrix equation. In the WBL, after one neglects the energy dependence of the linewidth function, the self-energy $\Sigma^R(t_1, t_2)$ becomes proportional to a delta function $\delta(t_1 - t_2)$, hence $G^R(t, t')$ can be solved afterward [4, 5, 7].

To solve the problem exactly without relying on the WBL, we define [4, 5]

$$A_\alpha(\epsilon, t) \equiv \int_{-\infty}^t dt' e^{i\epsilon(t-t')} e^{i \int_{t'}^t dt_1 \Delta_\alpha(t_1)} G^R(t, t'). \quad (3)$$

From the Keldysh equation and the expression for the lesser self-energy [5],

$$\Sigma^<(t_1, t_2) = \sum_\alpha \int \frac{d\omega}{2\pi} e^{-i\omega(t_1-t_2)} e^{i \int_{t_1}^{t_2} dt_3 \Delta_\alpha(t_3)} f(\omega) \Gamma_\alpha(\omega),$$

one can straightforwardly show that Eq. (2) takes the form

$$J_\alpha(t) = -2e \int \frac{d\epsilon}{2\pi} \text{Im Tr} \{ \Gamma_\alpha(\epsilon) [\Psi_\alpha(\epsilon, t) + f(\epsilon) A_\alpha(\epsilon, t)] \}, \quad (4)$$

where we have defined

$$\Psi_\alpha(\epsilon, t) \equiv i \sum_\beta \int \frac{d\epsilon'}{2\pi} e^{i(\epsilon-\epsilon')t} f(\epsilon') A_\beta(\epsilon', t) \Gamma_\beta(\epsilon')$$

$$\times \int_{-\infty}^t dt' e^{-i(\epsilon-\epsilon')t'} e^{i \int_{t'}^t dt_1 [\Delta_\alpha(t_1) - \Delta_\beta(t_1)]} A_\beta^\dagger(\epsilon', t').$$

Therefore, once $A_\alpha(\epsilon, t)$ can be found, the current is entirely determined.

To solve for $A_\alpha(\epsilon, t)$, we make use of an alternate version of the Dyson equation, namely that obtained by choosing only the time-dependent part of the Hamiltonian (1) as a perturbation, the unperturbed part being the time-independent terms. This way, the unperturbed Hamiltonian describes the LDL device at *equilibrium*, hence its physics is given by a time-translationally invariant Green's function $\tilde{G}^R(t - t')$. A standard expansion of the contour S -matrix along the Schwinger-Keldysh contour C [12, 13], followed by analytic continuation of the contour-ordered Green's function $G_{nm}(\tau, \tau') \equiv -i\langle T_C \{d_n(\tau) d_m^\dagger(\tau')\} \rangle$ to the real time axis according to the Langreth rules [14], yields the following alternate form of the Dyson equation,

$$G^R(t, t') = \tilde{G}^R(t - t') + \int dt_1 \tilde{G}^R(t - t_1) \Delta(t_1) G^R(t_1, t') + \int dt_1 \int dt_2 \tilde{G}^R(t - t_1) V^R(t_1, t_2) G^R(t_2, t'), \quad (5)$$

where we define a retarded potential [9] $V^R(t_1, t_2) \equiv \sum_\beta \left[\exp \left(-i \int_{t_2}^{t_1} dt' \Delta_\beta(t') \right) - 1 \right] \tilde{\Sigma}_\beta^R(t_1 - t_2)$ and $\tilde{\Sigma}_\beta^R$ is the equilibrium retarded self-energy due to lead β . Using Eq. (3) in the Dyson equation (5), we obtain the following integral equation for the quantity $A_\alpha(\epsilon, t)$:

$$A_\alpha(\epsilon, t) = \tilde{A}_\alpha(\epsilon, t) + \int dt' e^{i\epsilon(t-t')} e^{i \int_{t'}^t dt_1 \Delta_\alpha(t_1)} \tilde{G}^R(t - t') \times \Delta(t') A_\alpha(\epsilon, t') + \int dt_1 \int dt_2 e^{i\epsilon(t-t_2)} \times e^{i \int_{t_2}^{t_1} dt_3 \Delta_\alpha(t_3)} \tilde{G}^R(t - t_1) V^R(t_1, t_2) A_\alpha(\epsilon, t_2). \quad (6)$$

Here $\tilde{A}_\alpha(\epsilon, t) \equiv \int_{-\infty}^t dt' e^{i\epsilon(t-t')} e^{i \int_{t'}^t dt_1 \Delta_\alpha(t_1)} \tilde{G}^R(t - t')$ describes the equilibrium state and is therefore known. To solve Eq. (6), we need to specify the external fields $\Delta(t)$ and $\Delta_\alpha(t)$. Here we investigate a step function pulse applied at time $t = 0$, of the form $\Delta_{(\alpha)}(t) = \Delta_{(\alpha)}\theta(\pm t)$ where $\Delta_{(\alpha)}$ is a constant amplitude and the plus (minus) sign corresponds to an upward (downward) step.

Downward step pulse. This is the situation where a constant bias voltage with value Δ_α is sharply turned off at time $t = 0$ and remains off for subsequent times. For this case and from its definition, $V^R(t_1, t_2)$ vanishes when t_1 and t_2 are simultaneously greater than zero, as well as when $t_1 < t_2$ from the retarded self-energy. Equation (6) then takes the form

$$A_\alpha(\epsilon, t) = \tilde{A}_\alpha(\epsilon, t) + \int_{-\infty}^0 dt' e^{i\epsilon(t-t')} e^{i \int_{t'}^t dt_1 \Delta_\alpha(t_1)} \tilde{G}^R(t-t') \Delta A_\alpha(\epsilon, t') \\ + \left(\int_{-\infty}^0 dt_1 \int_{-\infty}^{t_1} dt_2 + \int_0^t dt_1 \int_{-\infty}^0 dt_2 \right) e^{i\epsilon(t-t_2)} e^{i \int_{t_2}^t dt_3 \Delta_\alpha(t_3)} \tilde{G}^R(t-t_1) V^R(t_1, t_2) A_\alpha(\epsilon, t_2). \quad (7)$$

We see from the limits of integration that while $A_\alpha(\epsilon, t)$ is required for $t > 0$ on the left-hand side of Eq. (7), only $A_\alpha(\epsilon, t < 0)$ is involved in the integrals on the right-hand side. This is an example of a Wiener-Hopf equation [15]. For our LDL device under this downward step pulse, $A_\alpha(\epsilon, t < 0)$ is actually known: for $t < 0$ the system is in steady-state under a constant bias Δ_α . Hence $A_\alpha(\epsilon, t < 0)$ is easily obtained from the known steady-state NEGF $\tilde{G}^R(t-t') \equiv G^R(t < 0, t' < 0)$. Equation (7) is therefore *not* an integral equation but an explicit expression for $A_\alpha(\epsilon, t)$ in terms of known quantities. Once the integrations are carried out by tedious but elementary algebra, one obtains the following exact expression:

$$A_\alpha(\epsilon, t) = \tilde{G}^R(\epsilon) + \int \frac{d\omega}{2\pi i} \frac{e^{-i(\omega-\epsilon)t} \tilde{G}^R(\omega)}{\omega - \epsilon - \Delta_\alpha - i0^+} \left[\frac{\Delta_\alpha}{\omega - \epsilon - i0^+} + \left(\Delta - \sum_\beta \Delta_\beta \tilde{Y}_{\alpha\beta}^R(\omega, \epsilon) \right) \tilde{G}^R(\epsilon + \Delta_\alpha) \right], \quad (8)$$

where we define $\tilde{Y}_{\alpha\beta}^R(\omega, \omega') \equiv [\tilde{\Sigma}_\beta^R(\omega) - \tilde{\Sigma}_\beta^R(\omega' + \Delta_\alpha - \Delta_\beta)]/(\omega - \omega' - \Delta_\alpha + \Delta_\beta)$. Equation (8) is the first important result of this paper. With the explicit solution for $A_\alpha(\epsilon, t)$, the time-dependent current $J_\alpha(t)$ can be obtained without further difficulty from Eq. (4).

Upward step pulse. In this case, Eq. (6) takes the form

$$A_\alpha(\epsilon, t) = A'_\alpha(\epsilon, t) + \int_0^t dt' e^{i(\epsilon+\Delta_\alpha)(t-t')} \tilde{G}^R(t-t') \\ \times \Delta A_\alpha(\epsilon, t') + \int_0^t dt_1 \int_0^{t_1} dt_2 e^{i(\epsilon+\Delta_\alpha)(t-t_1)} \\ \times \tilde{G}^R(t-t_1) e^{i(\epsilon+\Delta_\alpha)(t_1-t_2)} V^R(t_1, t_2) A_\alpha(\epsilon, t_2),$$

where $A'_\alpha(\epsilon, t)$ is a known function that involves only $\tilde{A}_\alpha(\epsilon, t)$ and $A_\alpha(\epsilon, t < 0)$. This is a Volterra equation which has the form of a Laplace convolution product. It can thus be converted into an algebraic matrix equation by a Laplace transformation, so that $A_\alpha(\epsilon, t)$ is given by the following Bromwich integral:

$$A_\alpha(\epsilon, t) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} d\sigma e^{\sigma t} \\ \times (1 - F_\alpha(\epsilon, \sigma) [\Delta + U_\alpha(\epsilon, \sigma)])^{-1} A'_\alpha(\epsilon, \sigma),$$

where σ is the Laplace variable, and we define $A'_\alpha(\epsilon, \sigma) \equiv \mathcal{L}_{t \rightarrow \sigma}\{A'_\alpha(\epsilon, t)\}$, $F_\alpha(\epsilon, \sigma) \equiv \mathcal{L}_{t \rightarrow \sigma}\{e^{i(\epsilon+\Delta_\alpha)t} \tilde{G}^R(t)\}$ and

$U_\alpha(\epsilon, \sigma) \equiv \mathcal{L}_{t \rightarrow \sigma}\{e^{i(\epsilon+\Delta_\alpha)t} V^R(t)\}$ which are all known quantities. Finally, a detailed but straightforward calculation gives

$$A_\alpha(\epsilon, t) = e^{i\Delta_\alpha t} \tilde{G}^R(\epsilon) + \int_{C_\gamma} \frac{dz}{2\pi i} \frac{e^{-izt} \tilde{G}^R(\epsilon + z + \Delta_\alpha)}{z + \Delta_\alpha} \\ \times \left[\frac{\Delta_\alpha}{z} + \left(\Delta - \sum_\beta \Delta_\beta \tilde{Y}_{\alpha\beta}^R(\epsilon, \epsilon + z) \right) \tilde{G}^R(\epsilon) \right], \quad (9)$$

where we define the contour $C_\gamma : \infty + i\gamma \rightarrow -\infty + i\gamma$ in the complex z -plane. Equation (9) is the second important result of this work.

Examples. The above exact solutions, Eqs. (8,9), are valid for arbitrary noninteracting phase-coherent devices in the LDL configuration. As an concrete example, we now apply these results to a quantum dot (QD) with a single energy level ϵ_0 connected to two leads described by a Lorentzian linewidth function $\Gamma_\alpha(\epsilon) = \Gamma_\alpha^0 W^2/(\epsilon^2 + W^2)$, where Γ_α^0 is a constant linewidth amplitude and W is the bandwidth. After the integrals in Eqs. (8,9) are carried out by residue integration, the time-dependent current $J_\alpha(t)$ of Eq. (4) is then given by a single integral over all frequencies. This last integral can be easily done numerically as it contains $f(\epsilon)$ which has known poles at the fermionic Matsubara frequencies $i\omega_n = i(2n+1)\pi/\beta$.

In Fig. 1 we show the time-dependent current $J_L(t)$ through the left lead in response to a *downward* step pulse. At $t = 0$, energies in the left lead are lowered by $\Delta_L = 10\Gamma$ and the energy of the QD level is lowered by $\Delta = 5\Gamma$ where Γ is the total linewidth amplitude. For $W \gg \Gamma, \Delta_L, \Delta$, the WBL result is essentially correct. When W becomes comparable to other energy scales of the problem, the WBL is seen to be a poor approximation. The initial current $J_L(0)$ decreases as the linewidth function gets narrower since less states in the leads are available for transport. More importantly, the time-dependent current can increase following the bias turnoff (curves (iv) and (v) in Fig. 1), an interesting nonclassical behavior not displayed by the WBL current. A current increase after the bias is turned off was also observed in a previous numerical study [9]. Most importantly, for devices with smaller bandwidth, the WBL and the exact solution predict very different time scales of the current decay. The inset shows an interesting oscillatory behavior, not captured by the WBL, for a narrow band $W = 0.25\Gamma$ misaligned with the resonant level $\epsilon_0 = -0.3\Gamma$.

In Fig. 2 we show the time-dependent current $J_L(t)$ through the left lead in response to an *upward* step pulse. In this case, the single-particle energies $\epsilon_{k\alpha}$ and ϵ_0 are suddenly raised at $t = 0$. Here again, the WBL is seen to be accurate for $W \gg \Gamma, \Delta_L, \Delta$. However, interesting finite-bandwidth effects appear as bands in the leads get narrower. First of all, the asymptotic $t \rightarrow \infty$ current decreases with W , corresponding to the initial current decrease in the downward step situation discussed in the last paragraph. In addition, it is seen that a *positive* voltage pulse can drive an instantaneously *negative* current, as has been observed in the numerical work of Ref. [9]. For $W < \Delta, \Delta_L$, the current oscillates around a zero value: the pulse drives the resonant level ϵ_0 outside the band so that little current can flow through.

In summary, we have presented an exact solution for the time-dependent current through an arbitrary non-interacting phase-coherent device scattering region connected to external leads with arbitrary energy-dependent linewidth functions, in the physically relevant case of an upward or downward step function voltage pulse. The results are general and are valid for far from equilibrium transport situations. For a single-level QD with Lorentzian linewidth function, the WBL was seen to be a crude approximation to the exact solution in the case of narrow bands. Due to the finite-bandwidth effects, a number of nonclassical transient behaviors were found including a current increase following a downward pulse, a negative current driven by a positive upward pulse, and a vanishing asymptotic current for a finite positive bias pulse. The significance of our solution is the exactness of the results which give unambiguous nonequilibrium transient quantum transport dynamics. From a practical application point of view, our formalism gives the transient current in terms of steady-state NEGF that can be calculated by any technique used for steady-state transport such as those atomistic first principles techniques of Ref. 16.

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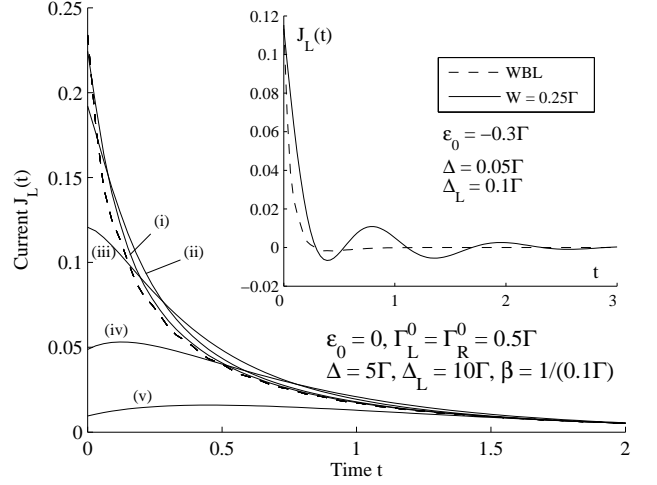


FIG. 1: Time-dependent current $J_L(t)$ through left lead in response to a downward step pulse for different bandwidths: dashed line, WBL ($W = \infty$); (i) $W = 20\Gamma$, (ii) $W = 10\Gamma$, (iii) $W = 5\Gamma$, (iv) $W = 2.5\Gamma$, and (v) $W = \Gamma$. The current is in units of $e\Gamma/\hbar$ and the time is in units of \hbar/Γ where $\Gamma = \Gamma_L^0 + \Gamma_R^0$ is the total linewidth amplitude. Parameters are taken the same as in Ref. 4. When $W = 100\Gamma$, the result was found (not shown) to be indistinguishable from the $W = \infty$ curve. The inset shows interesting oscillatory behavior, not captured by the WBL, for a narrow band $W = 0.25\Gamma$ misaligned with the resonant level $\epsilon_0 = -0.3\Gamma$.

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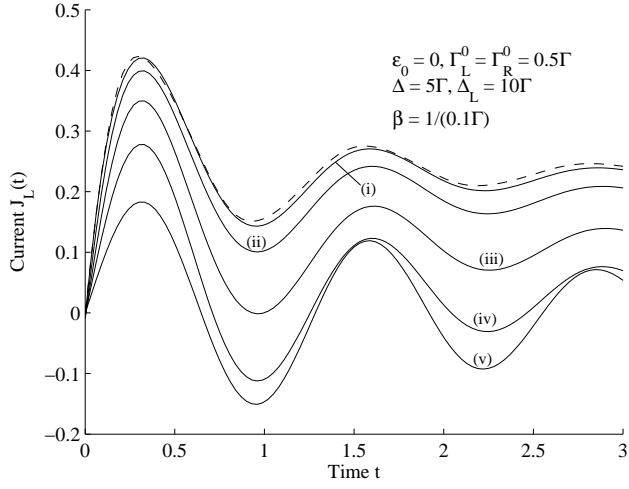


FIG. 2: Time-dependent current $J_L(t)$ through left lead in response to an upward step pulse for different bandwidths: dashed line, WBL ($W = \infty$); (i) $W = 20\Gamma$, (ii) $W = 10\Gamma$, (iii) $W = 5\Gamma$, (iv) $W = 2.5\Gamma$, and (v) $W = \Gamma$. Units and parameters are the same as in Fig. 1. Here again, the $W = 100\Gamma$ curve (not shown) is indistinguishable from the $W = \infty$ curve.